Mathematical Appendix[1]

1 Spaces, Trigonometry, and Vectors

1.1 Coordinates

To describe points quantitatively, we need to have a coordinate system. Constructing a coordinate system begins with choosing a point of space to be the *origin*. Sometimes the origin is chosen to make the equations especially simple. For example, the theory of the solar system would look more complicated if we put the origin anywhere but at the Sun. Strictly speaking, the location of the origin is arbitrary—put it anywhere—but once it is chosen, stick with the choice.

The next step is to choose three perpendicular axes. Again, their location is somewhat arbitrary as long as they are perpendicular. The axes are usually called x, y, and z but we can also call them x_1, x_2, and x_3. Such a system of axes is called a *Cartesian coordinate system*, as in Figure 1.1

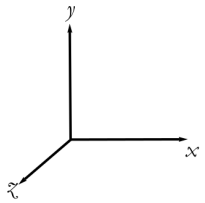

Figure 1.1: A three-dimensional Cartesian coordinate system.

We want to describe a certain point in space; call it P. It can be located by giving the x, y, z coordinates of the point. In other words, we identify the point P with the ordered triple of numbers (x, y, z) (see Figure 1.2).

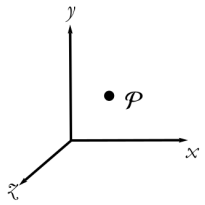

Figure 1.2: A point in Cartesian space.

The x coordinate represents the perpendicular distance of P from the plane defined by setting $x = 0$ (see Figure 1.3). The same is true for the y and z coordinates. Because the coordinates represent distances they are measured in units of length, such as meters.

When we study motion, we also need to keep track of time. Again we start with an origin—that is, the zero of time. We could pick the Big Bang to be the origin, or the birth of Jesus, or just the start of an experiment. But once we pick it, we don't change it.

Next we need to fix a direction of time. The usual convention is that positive times are to the future of the origin and negative times are to the past. We could do it the other way, but we won't.

[1] Adapted from Susskind, 2014 [1]; Vlugt, 2008 [2] & Gould, 2008 [3]

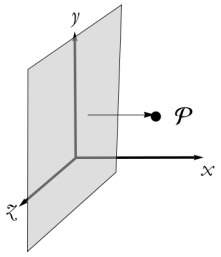

Figure 1.3: A plane defined by setting $x = 0$, and the distance to P along the x axis.

Finally, we need units for time. Seconds are the physicist's customary units, but hours, nanoseconds, or years are also possible. Once having picked the units and the origin, we can label any time by a number t.

There are two implicit assumptions about time in classical mechanics. The first is that time runs uniformly—an interval of 1 second has exactly the same meaning at one time as at another. For example, it took the same number of seconds for a weight to fall from the Tower of Pisa in Galileo's time as it takes in our time. One second meant the same thing then as it does now.

The other assumption is that times can be compared at different locations. This means that clocks located in different places can be synchronized. Given these assumptions, the four coordinates—x, y, z, t—define a *reference frame*. Any event in the reference frame must be assigned a value for each of the coordinates.

Given the function $f(t) = t^2$, we can plot the points on a coordinate system. We will use one axis for time, t, and another for the function, $f(t)$ (see Figure 1.4).

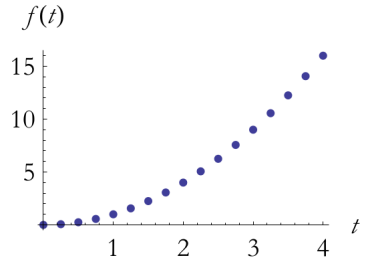

Figure 1.4: Plotting the points of $(t) = t^2$

We can also connect the dots with curves to fill in the spaces between the points (see Figure 5).

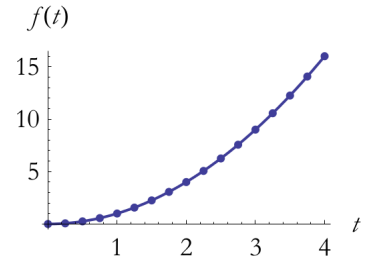

Figure 1.5: Joining the plotted points with curves.

In this way we can visualize functions.

1.2 TRIGONOMETRY

If you have not studied trigonometry, or if you studied it a long time ago, then this section is for you.

We use trigonometry in physics all the time; it is everywhere. So you need to be familiar with some of the ideas, symbols, and methods used in trigonometry. To begin with, in physics we do not generally use the degree as a measure of angle. Instead we use the *radian*; we say that there are 2π radians in 360°, or 1 radian = $\pi/180°$, thus $90° = \pi/2$ radians, and $30° = \pi/6$ radians. Thus a radian is about 57° (see Figure 1.6).

The trigonometric functions are defined in terms of properties of right triangles. Figure 7 illustrates the right triangle and its hypotenuse c, base b, and altitude a. The greek letter theta, θ, is defined to be the angle opposite the altitude, and the greek letter phi, ϕ, is defined to be the angle opposite the base.

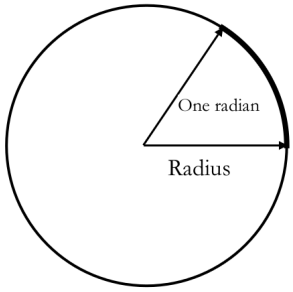

Figure 1.6: The radian as the angle subtended by an arc equal to the radius of the circle.

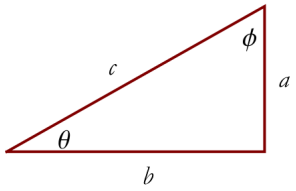

Figure 1.7: A right triangle with segments and angles indicated.

We define the functions sine (sin), cosine (cos), and tangent (tan), as ratios of the various sides according to the following relationships:

$$\sin\theta = \frac{a}{c}$$
$$\cos\theta = \frac{b}{c}$$
$$\tan\theta = \frac{a}{b} = \frac{\sin\theta}{\cos\theta}.$$

We can graph these functions to see how they vary (see Figures 1.8 through 1.10).

There are a couple of useful things to know about the trigonometric functions. The first is that we can draw a triangle within a circle, with the center of the circle located at the origin of a Cartesian coordinate system, as in Figure 1.11.

Here the line connecting the center of the circle to any point along its circumference forms the hypotenuse of a right triangle, and the horizontal and vertical components of the point are the base and altitude of that triangle. The position of a point can be specified by two coordinates, x and y, where

$$x = c\cos\theta$$

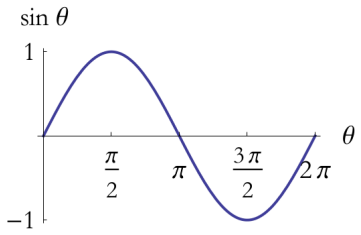

Figure 1.8: Graph of the sine function.

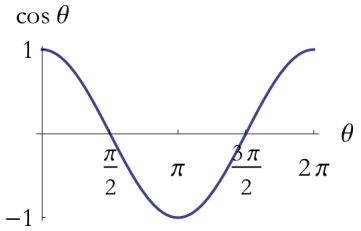

Figure 1.9: Graph of the cosine function.

and

$$y = c \sin\theta.$$

This is a very useful relationship between right triangles and circles.

Suppose a certain angle θ is the sum or difference of two other angles using the greek letters alpha, α, and beta, β, we can write this angle, θ, as $\alpha \pm \beta$. The trigonometric functions of $\alpha \pm \beta$ can be expressed in terms of the trigonometric functions of α and β.

$$\begin{aligned}
\sin(\alpha+\beta) &= \sin\alpha\cos\beta + \cos\alpha\sin\beta \\
\sin(\alpha-\beta) &= \sin\alpha\cos\beta - \cos\alpha\sin\beta \\
\cos(\alpha+\beta) &= \cos\alpha\cos\beta - \sin\alpha\sin\beta \\
\cos(\alpha-\beta) &= \cos\alpha\cos\beta + \sin\alpha\sin\beta
\end{aligned}$$

A final—very useful—identity is

$$\sin^2\theta + \cos^2\theta = 1. \tag{1.1}$$

(Notice the notation used here: $\sin^2\theta = \sin\theta\sin\theta$.) This equation is the Pythagorean theorem in disguise. If we choose the radius of the circle in Figure 1.11 to be 1, then the sides a and b are the sine and cosine of θ, and the hypotenuse is 1. Equation 1.1 is the familiar relation among the three sides of a right triangle: $a^2 + b^2 = c^2$.

1.3 VECTORS

Vector notation is another mathematical subject that we assume you have seen before, but—just to level the playing field—let's review vector methods in ordinary three-dimensional space.

A *vector* can be thought of as an object that has both a length (or *magnitude*) and a direction in space. An example is displacement. If an object is moved from some particular starting location, it is not enough to know how far it is moved in order to know where it winds up. One also has to know the direction of the

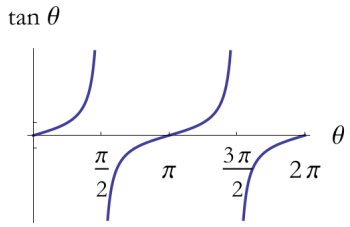

Figure 1.10: Graph of the tangent function.

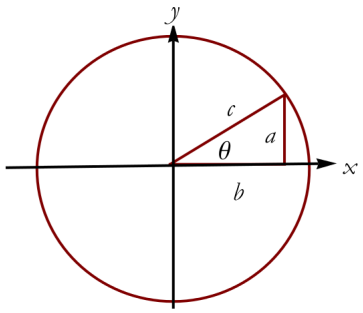

Figure 1.11: A right triangle drawn in a circle.

displacement. Displacement is the simplest example of a vector quantity. Graphically, a vector is depicted as an arrow with a length and direction, as shown in Figure 1.12.

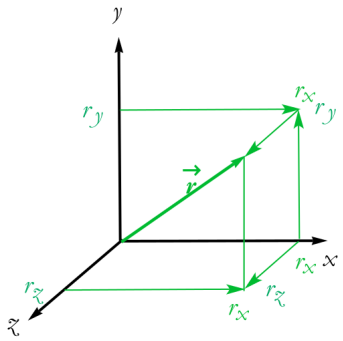

Figure 1.12: A vector $\vec{r}$ in Cartesian coordinates.

Symbolically vectors are represented by placing arrows over them. Thus the symbol for displacement is $\vec{r}$. The magnitude, or length, of a vector is expressed in absolute-value notation. Thus the length of $\vec{r}$ is denoted $|\vec{r}|$.

Here are some operations that can be done with vectors. First of all, you can multiply them by ordinary real numbers. When dealing with vectors you will often see such real numbers given the special name *scalar*. Multiplying by a positive number just multiplies the length of the vector by that number. But you can also multiply by a negative number, which reverses the direction of the vector. For example $-2\vec{r}$ is the vector that is twice as long as $\vec{r}$ but points in the opposite direction.

Vectors may be added. To add $\vec{A}$ and $\vec{B}$, place them as shown in Figure 1.13 to form a quadrilateral (this

way the directions of the vectors are preserved). The sum of the vectors is the length and angle of the diagonal.

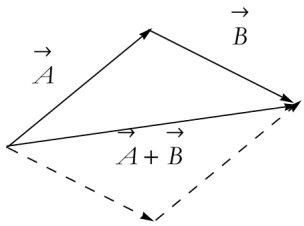

Figure 1.13: Adding vectors.

If vectors can be added and if they can be multiplied by negative numbers then they can be subtracted.

Vectors can also be described in component form. We begin with three perpendicular axes x, y, z. Next, we define three *unit vectors* that lie along these axes and have unit length. The unit vectors along the coordinate axes are called *basis vectors*. The three basis vectors for Cartesian coordinates are traditionally called $\hat{i}$, $\hat{j}$, and $\hat{k}$ (see Figure 14). More generally, we write $\hat{e_1}, \hat{e_2}$, and $\hat{e_3}$ when we refer to (x_1, x_2, x_3), where the symbol $\hat{}$(known as a carat) tells us we are dealing with unit (or basis) vectors. The basis vectors are useful because any vector $\vec{V}$ can be written in terms of them in the following way:

$$\vec{V} = V_x\hat{i} + V_y\hat{j} + V_z\hat{k}. \tag{1.2}$$

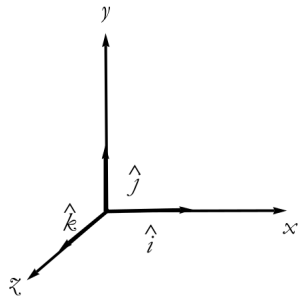

Figure 1.14: Basis vectors for a Cartesian coordinate system.

The quantities V_x, V_y, and V_z are numerical coefficients that are needed to add up the basis vectors to give $\vec{V}$. They are also called the *components* of $\vec{V}$. We can say that Eq. 1.2 is a *linear combination* of basis vectors. This is a fancy way of saying that we add the basis vectors along with any relevant factors. Vector components can be positive or negative. We can also write a vector as a list of its components—in this case (V_x, V_y, V_z). The magnitude of a vector can be given in terms of its components by applying the three-dimensional Pythagorean theorem.

$$\left|\vec{V}\right| = \sqrt{(V_x)^2 + (V_y)^2 + (V_z)^2} \tag{1.3}$$

We can multiply a vector $\vec{V}$ by a scalar, α, in terms of components by multiplying each component by α.

$$\alpha\vec{V} = (\alpha V_x, \alpha V_y, \alpha V_z)$$

We can write the sum of two vectors as the sum of the corresponding components.

$$\left(\vec{A}+\vec{B}\right)_x = (A_x + B_x)$$
$$\left(\vec{A}+\vec{B}\right)_y = (A_y + B_y)$$
$$\left(\vec{A}+\vec{B}\right)_z = (A_z + B_z).$$

Can we multiply vectors? Yes, and there is more than one way. One type of product—the cross product—gives another vector. For now, we will not worry about the cross product and only consider the other method, the *dot product*. The dot product of two vectors is an ordinary number, a scalar. For vectors $\vec{A}$ and $\vec{B}$ it is defined as follows:

$$\vec{A}\cdot\vec{B} = \left|\vec{A}\right|\left|\vec{B}\right|\cos\theta.$$

Here θ is the angle between the vectors. In ordinary language, the dot product is the product of the magnitudes of the two vectors and the cosine of the angle between them.

The dot product can also be defined in terms of components in the form

$$\vec{A}\cdot\vec{B} = A_xB_x + A_yB_y + A_zB_z.$$

This makes it easy to compute dot products given the components of the vectors.

An important property of the dot product is that it is zero if the vectors are *orthogonal* (perpendicular). Keep this in mind because we will have occasion to use it to show that vectors are orthogonal.

2 DIFFERENTIAL CALCULUS

In this book we will mostly be dealing with how various quantities change with time. Most of classical mechanics deals with things that change smoothly—*continuously* is the mathematical term—as time changes continuously. Dynamical laws that update a state will have to involve such continuous changes of time, unlike the stroboscopic changes of the first lecture. Thus we will be interested in functions of the independent variable t.

To cope, mathematically, with continuous changes, we use the mathematics of calculus. Calculus is about limits, so let's get that idea in place. Suppose we have a sequence of numbers, $l1, l2, l3, \ldots$, that get closer and closer to some value L. Here is an example: $0.9, 0.99, 0.999, 0.9999, \ldots$. The limit of this sequence is 1. None of the entries is equal to 1, but they get closer and closer to that value. To indicate this we write

$$\lim_{i\to\infty} l_i = L.$$

In words, L is the limit of l_i as i goes to infinity.

We can apply the same idea to functions. Suppose we have a function, $f(t)$, and we want to describe how it varies as t gets closer and closer to some value, say a. If $f(t)$ gets arbitrarily close to L as t tends to a, then we say that the limit of $f(t)$ as t approaches a is the number L. Symbolically,

$$\lim_{t\to a} f(t) = L.$$

Let $f(t)$ be a function of the variable t. As t varies, so will $f(t)$. Differential calculus deals with the rate of change of such functions. The idea is to start with $f(t)$ at some instant, and then to change the time by a little bit and see how much $f(t)$ changes. The rate of change is defined as the ratio of the change in f to the change in t. We denote the change in a quantity with the uppercase greek letter delta, Δ. Let the change in t be called Δt. (This is not $\Delta \times t$, this is a change in t.) Over the interval Δt, f changes from $f(t)$ to $f(t+\Delta t)$. The change in f, denoted Δf, is then given by

$$\Delta f = f(t+\Delta t) - f(t).$$

To define the rate of change precisely at time t, we must let Δt shrink to zero. Of course, when we do that Δf also shrinks to zero, but if we divide Δf by Δt, the ratio will tend to a limit. That limit is the derivative of $f(t)$ with respect to t,

$$\frac{df(t)}{dt} = \lim_{\Delta t\to 0} \frac{\Delta f}{\Delta t} = \lim_{\Delta t\to 0} \frac{f(t+\Delta t) - f(t)}{\Delta t}. \tag{2.1}$$

A rigorous mathematician might frown on the idea that $\frac{df(t)}{dt}$ is the ratio of two differentials, but you will rarely make a mistake this way.

Let's calculate a few derivatives. Begin with functions defined by powers of t. In particular, let's illustrate the method by calculating the derivative of $f(t) = t^2$. We apply Eq. 2.1 and begin by defining $f(t+\Delta t)$:

$$f(t+\Delta t) = (t+\Delta t)^2.$$

We can calculate $(t+\Delta t)^2$ by direct multiplication or we can use the binomial theorem. Either way,

$$f(t+\Delta t) = t^2 + 2t\Delta t + \Delta t^2.$$

We now subtract $f(t)$:

$$f(t+\Delta t) - f(t) = t^2 + 2t\Delta t + \Delta t^2 - t^2$$

$$= 2t\Delta t + \Delta t^2.$$

The next step is to divide by Δt:

$$\begin{aligned}\frac{f(t+\Delta t)-f(t)}{\Delta t} &= \frac{2t\Delta t+\Delta t^2}{\Delta t}\\ &= 2t+\Delta t.\end{aligned}$$

Now it's easy to take the limit $\Delta t \to 0$. The first term does not depend on Δt and survives, but the second term tends to zero and just disappears. This is something to keep in mind: Terms of higher order in Δt can be ignored when you calculate derivatives. Thus

$$\lim_{\Delta t\to 0}\frac{f(t+\Delta t)-f(t)}{\Delta t} = 2t$$

So the derivative of t^2 is

$$\frac{d(t^2)}{dt} = 2t$$

Next let us consider a general power, $f(t) = t^n$. To calculate its derivative, we have to calculate $f(t+\Delta t) = (t+\Delta t)^n$. Here, high school algebra comes in handy: The result is given by the binomial theorem. Given two numbers, a and b, we would like to calculate $(a+b)^n$. The binomial theorem gives

$$\begin{aligned}(a+b)^n = a^n + na^{n-1}b + \frac{n(n-1)}{2}a^{n-2}b^2 +\\ \frac{n(n-1)(n-2)}{3}a^{n-3}b^3 +\\ \cdots + b^n\end{aligned}$$

How long does the expression go on? If n is an integer, it eventually terminates after $n+1$ terms. But the binomial theorem is more general than that; in fact, n can be any real or complex number. If n is not an integer, however, the expression never terminates; it is an infinite series. Happily, for our purposes, only the first two terms are important.

To calculate $(t+\Delta t)^n$, all we have to do is plug in $a = t$ and $b = \Delta t$ to get

$$\begin{aligned}f(t+\Delta t) &= (t+\Delta t)^n\\ &= t^n + nt^{n-1}\Delta t + \cdots.\end{aligned}$$

All the terms represented by the dots shrink to zero in the limit, so we ignore them.

Now subtract $f(t)$ (or t^n),

$$\begin{aligned}\Delta f &= f(t+\Delta t) - f(t)\\ &= t^n + nt^{n-1}\Delta t +\\ &\frac{n(n-1)}{2}t^{n-2}\Delta t^2 + \cdots - t^n\\ &= nt^{n-1}\Delta t +\\ &\frac{n(n-1)}{2}t^{n-2}\Delta t^2 + \cdots.\end{aligned}$$

Now divide by Δt,

$$\frac{\Delta f}{\Delta t} = nt^{n-1} + \frac{n(n-1)}{2}t^{n-2}\Delta t + \cdots.$$

and let $\Delta t \to 0$. The derivative is then

$$\frac{d(t^n)}{dt} = nt^{n-1}.$$

One important point is that this relation holds even if n is not an integer; n can be any real or complex number.

Here are some special cases of derivatives: If $n = 0$, then $f(t)$ is just the number 1. The derivative is zero—this is the case for any function that does't change. If $n = 1$, then $f(t) = t$ and the derivative is 1—this is always true when you take the derivative of something with respect to itself. Here are some derivatives of powers

$$\begin{aligned}
\frac{d(t^2)}{dt} &= 2t \\
\frac{d(t^3)}{dt} &= 3t^2 \\
\frac{d(t^4)}{dt} &= 4t^3 \\
\frac{d(t^n)}{dt} &= nt^{n-1}.
\end{aligned}$$

For future reference, here are some other derivatives:

$$\begin{aligned}
\frac{d(\sin\ t)}{dt} &= \cos\ t \\
\frac{d(\cos\ t)}{dt} &= -\sin\ t \\
\frac{d(e^t)}{dt} &= e^t \\
\frac{d(\log(t))}{dt} &= \frac{1}{t}.
\end{aligned} \tag{2.2}$$

One comment about the third formula in Eq. 2.2, $\frac{d(e^t)}{dt} = e^t$. The meaning of e^t is pretty clear if t is an integer. For example, $e^3 = e \times e \times e$. Its meaning for non-integers is not obvious. Basically, e^t is defined by the property that its derivative is equal to itself. So the third formula is really a definition.

There are a few useful rules to remember about derivatives. You can prove them all if you want a challenging exercise. The first is the fact that the derivative of a constant is always 0. This makes sense; the derivative is the rate of change, and a constant never changes, so

$$\frac{dc}{dt} = 0.$$

The derivative of a constant times a function is the constant times the derivative of the function:

$$\frac{d(cf)}{dt} = c\frac{df}{dt}.$$

Suppose we have two functions, $f(t)$ and $g(t)$. Their sum is also a function and its derivative is given by

$$\frac{d(f+g)}{dt} = \frac{d(f)}{dt} + \frac{d(g)}{dt}.$$

This is called the *sum rule*.

Their product of two functions is another function, and its derivative is

$$\frac{d(fg)}{dt} = f(t)\frac{d(g)}{dt} + g(t)\frac{d(f)}{dt}.$$

Not surprisingly, this is called the *product rule*.

Next, suppose that $g(t)$ is a function of t, and $f(g)$ is a function of g. That makes f an *implicit function* of t. If you want to know what f is for some t, you first compute $g(t)$. Then, knowing g, you compute $f(g)$. It's easy to calculate the t-derivative of f:

$$\frac{df}{dt} = \frac{df}{dg}\frac{dg}{dt}.$$

This is called the *chain rule*. This would obviously be true if the derivatives were really ratios; in that case, the dg's would cancel in the numerator and denominator. In fact, this is one of those cases where the naive answer is correct. The important thing to remember about using the chain rule is that you invent an intermediate function, $g(t)$, to simplify $f(t)$ making it $f(g)$. For example, if

$$f(t) = \ln\ t^3$$

and we need to find $\frac{df}{dt}$, then the t^3 inside the logarithm might be a problem. Therefore, we invent the intermediate function $g = t^3$, so we have $f(g) =$
$ln\ g$. We can then apply the chain rule.

$$\frac{df}{dt} = \frac{df}{dg}\frac{dg}{dt}.$$

We can use our differentiation formulas to note that $\frac{df}{dg} = \frac{1}{g}$ and $\frac{dg}{dt} = 3t^2$, so

$$\frac{df}{dt} = \frac{3t^2}{g}.$$

We can substitute $g = t^3$, to get

$$\frac{df}{dt} = \frac{3t^2}{t^3} = \frac{3}{t}.$$

That is how to use the chain rule.

Using these rules, you can calculate a lot of derivatives. That's basically all there is to differential calculus.

3 INTEGRAL CALCULUS

Differential calculus has to do with rates of change. Integral calculus has to do with sums of many tiny incremental quantities. It's not immediately obvious that these have anything to do with each other, but they do.

We begin with the graph of a function $f(t)$, as in Figure 3.1.

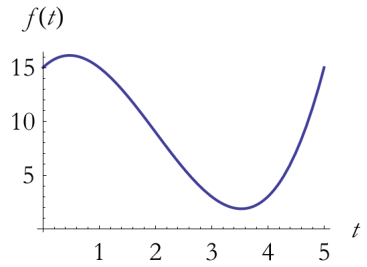

Figure 3.1: The behavior of $f(t)$.

The central problem of integral calculus is to calculate the area under the curve defined by $f(t)$. To make the problem well defined, we consider the function between two values that we call *limits of integration*, $t = a$ and $t = b$. The area we want to calculate is the area of the shaded region in Figure 3.2.

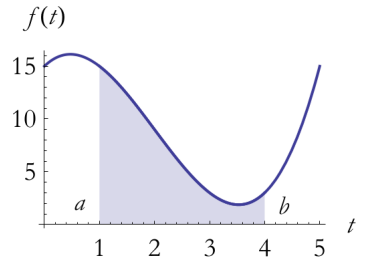

Figure 3.2: The limits of integration.

In order to do this, we break the region into very thin rectangles and add their areas (see Figure 3.3).

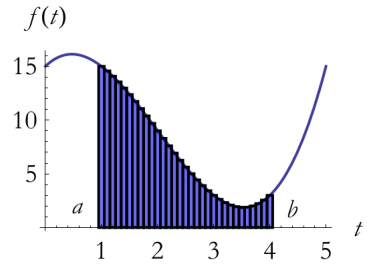

Figure 3.3: An illustration of integration.

Of course this involves an approximation, but it becomes accurate if we let the width of the rectangles tend to zero. In order to carry out this procedure, we first divide the interval between $t = a$ and $t = b$ into a number, N, of subintervals—each of width Δt. Consider the rectangle located at a specific value of t. The

width is Δt and the height is the local value of $f(t)$. It follows that the area of a single rectangle, δA, is

$$\delta A = f(t)\Delta t.$$

Now we add up all the areas of the individual rectangles to get an approximation to the area that we are seeking. The approximate answer is

$$A = \sum_i f(t_i)\Delta t$$

where the uppercase greek letter sigma, Σ, indicates a sum of successive values defined by i. So, if $N = 3$, then

$$\begin{aligned} A &= \sum_i^3 f(t_i)\Delta t \\ &= f(t_1)\Delta t + f(t_2)\Delta t + f(t_3)\Delta t. \end{aligned}$$

Here t_i is the position of the ith rectangle along the t axis.

To get the exact answer, we take the limit in which Δt shrinks to zero and the number of rectangles increases to infinity. That defines the *definite integral* of $f(t)$ between the limits $t = a$ and $t = b$. We write this as

$$A = \int_a^b f(t)\,dt = \lim_{\Delta t \to 0} \sum_i f(t_i)\Delta t.$$

The integral sign, called *summa*, $\int$, replaces the summation sign, and—as in differential calculus—Δt is replaced by dt. The function $f(t)$ is called the *integrand*.

Let's make a notational change and call one of the limits of integration T. In particular, replace b by T and consider the integral

$$\int_a^T f(t)\,dt$$

where we are going to think of T as a variable instead of as a definite value of t. In this case, this integral defines a function of T, which can take on any value of t. The integral is a function of T because it has a definite value for each value of T.

$$F(T) = \int_a^T f(t)\,dt.$$

Thus a given function $f(t)$ defines a second function $F(T)$. We could also let a vary, but we won't. The function $F(T)$ is called the *indefinite integral* of $f(t)$. It is indefinite because instead of integrating from a fixed value to a fixed value, we integrate to a variable. We usually write such an integral without limits of integration,

$$F(t) = \int f(t)\,dt. \tag{3.1}$$

The *fundamental theorem of calculus* is one of the simplest and most beautiful results in mathematics. It asserts a deep connection between integrals and derivatives. What it says is that if $F(T) = \int f(t)\,dt$, then

$$f(t) = \frac{dF(t)}{dt}.$$

To see this, consider a small incremental change in T from T to $T + \Delta t$. Then we have a new integral,

$$F(T + \Delta t) = \int_a^{T+\Delta t} f(t)\,dt.$$

In other words, we have added one more rectangle of width Δt at $t = T$ to the area shaded in Figure 3.3. In fact, the difference $F(T+\Delta t) - F(T)$ is just the area of that extra rectangle, which happens to be $f(T)\Delta t$, so

$$F(T+\Delta t) - F(T) = f(T)\Delta t.$$

Dividing by Δt,

$$\frac{F(T+\Delta t) - F(T)}{\Delta t} = f(T)$$

we obtain the fundamental theorem connecting F and f, when we take the limit where $\Delta t \to 0$:

$$\frac{dF}{dT} = \lim_{\Delta t \to 0} \frac{F(T+\Delta t) - F(T)}{\Delta t} = f(T).$$

We can simplify the notation by ignoring the difference between t and T,

$$\frac{dF}{dt} = f(t).$$

In other words, the processes of integration and differentiation are reciprocal: The derivative of the integral is the original integrand.

Can we completely determine $F(t)$ knowing that its derivative is $f(t)$? Almost, but not quite. The problem is that adding a constant to $F(t)$ does not change its derivative. Given $f(t)$, its indefinite integral is ambiguous, but only up to adding a constant.

To see how the fundamental theorem is used, let's work out some indefinite integrals. Let's find the integral of a power $f(t) = t^n$. Consider,

$$F(t) = \int f(t)\,dt.$$

It follows that

$$f(t) = \frac{dF(t)}{dt}$$

or

$$t^n = \frac{dF(t)}{dt}.$$

All we need to do is find a function F whose derivative is t^n, and that is easy.

In the last chapter we found that for any m,

$$\frac{d(t^m)}{dt} = mt^{m-1}.$$

If we substitute $m = n+1$, this becomes

$$\frac{d(t^{n+1})}{dt} = (n+1)\,t^n$$

or, dividing by $n+1$,

$$\frac{d(t^{n+1}/n+1)}{dt} = t^n.$$

Thus we find that t^n is the derivative of $\frac{t^{n+1}}{n+1}$. Substituting the relevant values, we get

$$F(t) = \int t^n\,dt = \frac{t^{n+1}}{n+1}.$$

The only thing missing is the ambiguous constant that we can add to F. We should write

$$F(t) = \int t^n \, dt = \frac{t^{n+1}}{n+1} + c.$$

where c is a constant that has to be determined by other means.

The ambiguous constant is closely related to the ambiguity in choosing the other endpoint of integration that we earlier called a. To see how a determines the ambiguous constant c, let's consider the integral

$$\int_a^T f(t) \, dt.$$

in the limit where the two limits of integration come together—that is, $T = a$. In this case, the integral has to be zero. You can use that fact to determine c.

In general, the fundamental theorem of calculus is written

$$\int_a^b f(t) \, dt = F(t)\Big|_a^b = F(b) - F(a). \tag{3.2}$$

Another way to express the fundamental theorem is by a single equation:

$$\int \frac{df}{dt} \, dt = f(t) + c. \tag{3.3}$$

In other words, integrating a derivative gives back the original function (up to the usual ambiguous constant). Integration and differentiation undo each other.

Here are some integration formulas:

$$\int c \, dt = ct$$

$$\int c f(t) \, dt = c \int f(t) \, dt$$

$$\int t \, dt = \frac{t^2}{2} + c$$

$$\int t^2 \, dt = \frac{t^3}{3} + c$$

$$\int t^n \, dt = \frac{t^{n+1}}{n+1} + c$$

$$\int \sin \, t \, dt = -\cos \, t + c$$

$$\int \cos \, t \, dt = \sin \, t + c$$

$$\int e^t \, dt = e^t$$

$$\int \frac{dt}{t} = \ln \, t + c$$

$$\int [f(t) \pm g(t)] \, dt = \int f(t) \, dt \pm \int g(t) \, dt.$$

3.1 INTEGRATION BY PARTS

There are some tricks to doing integrals. One trick is to look them up in a table of integrals. Another is to learn to use *Mathematica*. But if you're on your own and you don't recognize the integral, the oldest trick in the book is *integration by parts*. It's just the reverse of using the product rule for differentiation. Recall that to differentiate a function, which itself is a product of two functions, you use the following rule:

$$\frac{d[f(x)g(x)]}{dx} = f(x)\frac{dg(x)}{dx} + g(x)\frac{df(x)}{dx}.$$

Now let's integrate both sides of this equation between limits a and b.

$$\int_a^b \frac{d[f(x)g(x)]}{dx} = \int_a^b f(x)\frac{dg(x)}{dx} + \int_a^b g(x)\frac{df(x)}{dx}$$

The left side of the equation is easy. The integral of a derivative (the derivative of fg) is just the function itself. The left side is

$$f(b)g(b) - f(a)g(a)$$

which we often write in the form

$$f(x)g(x)|_a^b.$$

Now let's subtract one of the two integrals on the right side and shift it to the left side.

$$f(x)g(x)|_a^b - \int_a^b f(x)\frac{dg(x)}{dx} = \int_a^b g(x)\frac{df(x)}{dx}. \tag{3.4}$$

Suppose we have some integral that we don't recognize, but we notice that the integrand happens to be a product of a function $f(x)$ and the derivative of another function $g(x)$. In other words, after some inspection, we see that the integral has the form of the right side of Eq. 3.4, but we don't know how to do it. Sometimes we are lucky and recognize the integral on the left side of the equation.

Let's do an example. Suppose the integral that we want to do is

$$\int_0^{\frac{\pi}{2}} x \cos x \, dx.$$

That's not in our list of integrals. But notice that

$$\cos x = \frac{d \sin x}{dx}$$

so the integral is

$$\int_0^{\frac{\pi}{2}} x\frac{d \sin x}{dx} dx.$$

Equation 3.4 tells us that this integral is equal to

$$x \sin x|_0^{\frac{\pi}{2}} - \int_0^{\frac{\pi}{2}} \frac{dx}{dx} \sin x \, dx$$

or just

$$\frac{\pi}{2} \sin\frac{\pi}{2} - \int_0^{\frac{\pi}{2}} \sin x \, dx.$$

Now it's easy. The integral $\int \sin x \, dx$ is on our list: it's just $\cos x$. I'll leave the rest to you.

You might wonder how often this trick works. The answer is quite often, but certainly not always. Good luck.

4 Partial Differentiation

4.1 Partial Derivatives

The calculus of multivariable functions is a straightforward generalization of single-variable calculus. Instead of a function of a single variable t, consider a function of several variables. To illustrate, let's call the variables x, y, z, although these don't have to stand for the coordinates of ordinary space. Moreover, there can be more or fewer then three. Let us also consider a function of these variables, $V(x, y, z)$. For every value of x, y, z, there is a unique value of $V(x, y, z)$ that we assume varies smoothly as we vary the coordinates.

Multivariable differential calculus revolves around the concept of *partial derivatives*. Suppose we are examining the neighborhood of a point x, y, z, and we want to know the rate at which V varies as we change x while keeping y and z fixed. We can just imagine that y and z are fixed parameters, so the only variable is x. The derivative of V is then defined by

$$\frac{dV}{dx} = \lim_{\Delta x \to 0} \frac{\Delta V}{\Delta x} \tag{4.1}$$

where ΔV is defined by

$$\Delta V = V([x + \Delta x], y, z) - V(x, y, z). \tag{4.2}$$

Note that in the definition of ΔV, only x has been shifted; y and z are kept fixed.

The derivative defined by Eq. 4.1 and Eq. 4.2 is called the *partial derivative* of V with respect to x and is denoted

$$\frac{\partial V}{\partial x}$$

or, when we want to emphasize that y and z are kept fixed,

$$\left(\frac{\partial V}{\partial x}\right)_{y,z}.$$

By the same method we can construct the partial derivative with respect to either of the other variables:

$$\frac{\partial V}{\partial y} = \lim_{\Delta y \to 0} \frac{\Delta V}{\Delta y}.$$

A shorthand notation for the partial derivatives of V with respect to y is

$$\frac{\partial V}{\partial y} = \partial_y V.$$

Multiple derivatives are also possible. If we think of $\frac{\partial V}{\partial x}$ as itself being a function of x, y, z, then it can be differentiated. Thus we can define the second-order partial derivative with respect to x:

$$\frac{\partial^2 V}{\partial x^2} = \partial_x \left(\frac{\partial V}{\partial x}\right) = \partial_{x,x} V.$$

Mixed partial derivatives also make sense. For example, one can differentiate $\partial_y V$ with respect to x:

$$\frac{\partial^2 V}{\partial x \partial y} = \partial_x \left(\frac{\partial V}{\partial y}\right) = \partial_{x,y} V.$$

It's an interesting and important fact that the mixed derivatives do not depend on the order in which the derivatives are carried out. In other words,

$$\frac{\partial^2 V}{\partial x \partial y} = \frac{\partial^2 V}{\partial y \partial x}$$

4.2 Stationary Points and Minimizing Functions

Let's look at a function of y that we will call F (see Figure 4.1).

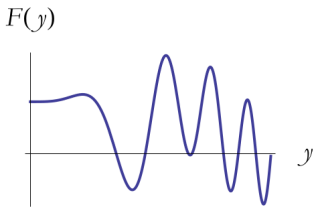

Figure 4.1: Plot of the function $F(y)$.

Notice that there are places on the curve where a shift in y in either direction produces only an upward shift in F. These points are called *local minima*. In Figure 4.2 we have added dots to indicate the local minima.

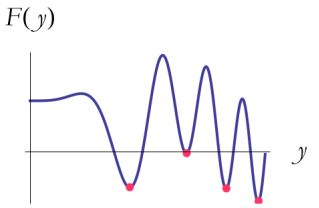

Figure 4.2: Local minima.

For each local minimum, when you go in either direction along y, you begin to rise above the dot in $F(y)$. Each dot is at the bottom of a little depression. The global minimum is the lowest possible place on the curve.

One condition for a local minimum is that the derivative of the function with respect to the independent variable at that point is zero. This is a necessary condition, but not a sufficient condition. This condition defines any *stationary point*,

$$\frac{d}{dy}F(y) = 0.$$

The second condition tests to see what the character of the stationary point is by examining its second derivative. If the second derivative is larger than 0, then all points nearby will be above the stationary point, and we have a *local minimum*:

$$\frac{d^2}{d^2y}F(y) > 0.$$

If the second derivative is less than 0, then all points nearby will be below the stationary point, and we have a *local maximum*:

$$\frac{d^2}{d^2y}F(y) < 0.$$

See Figure 4.3 for examples of local maxima.

If the second derivative is equal to 0, then the derivative changes from positive to negative at the stationary point, which we call a *point of inflection*:

$$\frac{d^2}{d^2y}F(y) = 0.$$

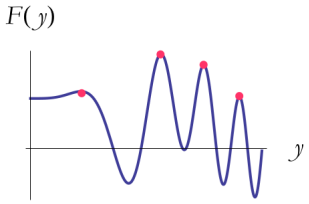

Figure 4.3: Local maxima.

See Figure 4.4 for an example of a point of inflection.

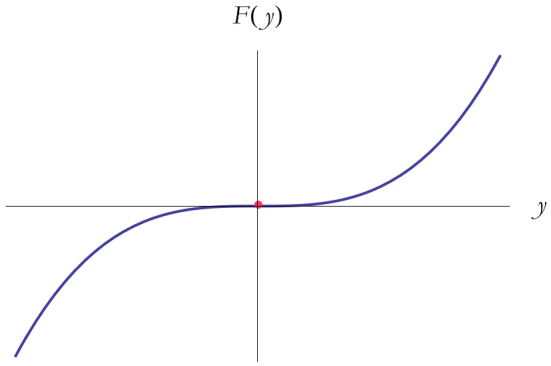

Figure 4.4: Point of inflection.

These are collectively the results of a *second-derivative test.*

4.3 Stationary Points in Higher Dimensions

Local maxima, local minima, and other stationary points can happen for functions of more than one variable. Imagine a hilly terrain. The altitude is a function that depends on the two coordinates—let's say latitude and longitude. Call it $A(x, y)$. The tops of hills and the bottoms of valleys are local maxima and minima of $A(x, y)$. But they are not the only places where the terrain is locally horizontal. Saddle points occur between two hills. You can see some examples in Figure 4.5.

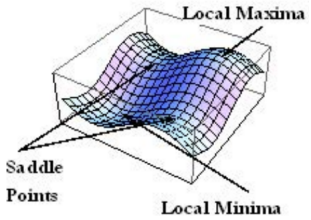

Figure 4.5: A function of several variables.

The very tops of hills are places where no matter which way you move, you soon go down. Valley bottoms are the opposite; all directions lead up. But both are places where the ground is level.

There are other places where the ground is level. Between two hills you can find places called saddles.

Saddle points are level, but along one axis the altitude quickly increases in either direction. Along another perpendicular direction the altitude decreases. All of these are called stationary points.

Let's take a slice along the x axis through our space so that the slice passes through a local minimum of A, see Figure 4.6.

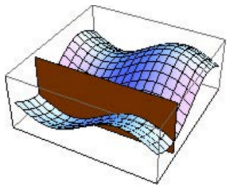

Figure 4.6: A slice along the x axis.

It's apparent that at the minimum, the derivative of A with respect to x vanishes, we write this:

$$\frac{\partial A}{\partial x} = 0.$$

On the other hand, the slice could have been oriented along the y axis, and we would then conclude that

$$\frac{\partial A}{\partial y} = 0.$$

To have a minimum, or for that matter to have any stationary point, both derivatives must vanish. If there were more directions of space in which A could vary, then the condition for a stationary point is given by:

$$\frac{\partial A}{\partial x_i} = 0. \tag{4.3}$$

for all x_i.

There is a shorthand for summarizing these equations. Recall that the change in a function when the point x is varied a little bit is given by

$$\delta A = \sum_i \frac{\partial A}{\partial x_i} \delta x_i.$$

The set of Equations 4.3 are equivalent to the condition that

$$\delta A = 0 \tag{4.4}$$

for any small variation of x.

Suppose we found such a point. How do we tell whether it is a maximum, a minimum, or a saddle. The answer is a generalization of the criterion for a single variable. We look at the second derivatives. But there are several second derivatives. For the case of two dimensions, we have

$$\frac{\partial^2 A}{\partial x^2},$$

$$\frac{\partial^2 A}{\partial y^2},$$

$$\frac{\partial^2 A}{\partial x \partial y},$$

and

$$\frac{\partial^2 A}{\partial y \partial x},$$

the last two being the same.

These partial derivatives are often arranged into a special matrix called the *Hessian matrix*.

$$H = \begin{pmatrix} \frac{\partial^2 A}{\partial x^2} & \frac{\partial^2 A}{\partial x \partial y} \\ \frac{\partial^2 A}{\partial y \partial x} & \frac{\partial^2 A}{\partial y^2} \end{pmatrix}.$$

Important quantities, called the determinant and the trace, can be made out of such a matrix. The determinant is given by

$$\text{Det } H = \frac{\partial^2 A}{\partial x^2}\frac{\partial^2 A}{\partial y^2} - \frac{\partial^2 A}{\partial y \partial x}\frac{\partial^2 A}{\partial x \partial y}$$

and the trace is given by

$$\text{Tr } H = \frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2}.$$

Matrices, determinants, and traces may not mean much to you beyond these definitions, but they will if you follow these lectures to the next subject—quantum mechanics. For now, all you need is the definitions and the following rules.

If the determinant and the trace of the Hessian is positive then the point is a local minimum.

If the determinant is positive and the trace negative the point is a local maximum.

If the determinant is negative, then irrespective of the trace, the point is a saddle point.

However: One caveat, these rules specifically apply to functions of two variables. Beyond that, the rules are more complicated. None of this is obvious for now, but it still enables you to test various functions and find their different stationary points. Let's take an example. Consider

$$F(x, y) = \sin\, x + \sin\, y.$$

Differentiating, we get

$$\frac{\partial F}{\partial x} = \cos\, x$$

$$\frac{\partial F}{\partial y} = \cos\, y.$$

Take the point $x = \frac{\pi}{2}, y = \frac{\pi}{2}$. Since $\cos\frac{\pi}{2} = 0$, both derivatives are zero and the point is a stationary point.

Now, to find the type of stationary point, compute the second derivatives. The second derivatives are

$$\frac{\partial^2 F}{\partial x^2} = -\sin\, x$$

$$\frac{\partial^2 F}{\partial x^y} = -\sin\ y$$

$$\frac{\partial^2 F}{\partial x \partial y} = 0$$

$$\frac{\partial^2 F}{\partial y \partial x} = 0$$

Since $\sin \frac{\pi}{2} = 1$ we see that both the determinant and the trace of the Hessian are positive. The point is therefore a minimum.

5 ESSENTIAL MATHEMATICS

Here we briefly review the mathematics that is most frequently used. Below, we give neither a proper derivation nor a proof of any of the results that we quote. However, in some cases we do provide a non-rigorous "justification". We assume that the reader is familiar with the most common functions and algebraic manipulations.

5.1 PROPERTIES OF $\ln x$ AND $\exp x$

The essential properties of logarithms and exponentials are - of course - well known $\cdots$ but still often forgotten. Often, we use $\exp(x)$ for e^x.

$$\ln(a \times b) = \ln a + \ln b \tag{5.1}$$

$$\ln(a/b) = \ln a - \ln b \tag{5.2}$$

$$\ln(a^b) = b \times \ln a \tag{5.3}$$

$$^g\log(a) = \ln(a)/\ln(g) \tag{5.4}$$

$$\exp(a+b) = (\exp a) \times (\exp b) \tag{5.5}$$

$$\exp(\ln(a)) = a \tag{5.6}$$

$$(\exp(a))^x = \exp(ax) \tag{5.7}$$

5.2 CHAIN RULE

When differentiating a function $F(u)$, where $u(x)$ is a function of the independent variable x, we can use the so-called chain rule

$$\frac{\partial F(u(x))}{\partial x} = \frac{\partial F(u)}{\partial u} \times \frac{\partial u(x)}{\partial u} \tag{5.8}$$

More generally, if $F(u)$ is a function of u and u is a function of $v \cdots$ and y is a function of z, then

$$\frac{\partial F}{\partial z} = \frac{\partial F(u)}{\partial u} \times \frac{\partial u(v)}{\partial v} \times \frac{\partial v(w)}{\partial w} \times \cdots \times \frac{\partial y(z)}{\partial z}$$

5.3 DERIVATIVE OF $\exp(ax)$ AND $\ln(x)$

The derivative of $\exp(ax)$:

$$\frac{\partial \exp(ax)}{\partial x} = a \exp(ax) \tag{5.9}$$

This result can easily be derived from the definition of $\exp(ax)$:

$$\exp(ax) = \sum_{n=0}^{\infty} \frac{(ax)^n}{n!} = \lim_{n\to\infty} (1 + \frac{ax}{n})^n \tag{5.10}$$

Conversely, the primitive function of $\exp(ax)$ is $a^{-1}\exp(ax)$. The derivative of $\ln x$ with respect to x is

$$\frac{\partial \ln x}{\partial x} = \frac{1}{x} \tag{5.11}$$

This is easily derived from Eq. 5.9. If $y = \ln x$, then $x = \exp(y)$, hence

$$\frac{\partial \ln x}{\partial x} = \frac{\partial y}{\partial \exp y} = \frac{1}{\exp y} = \frac{1}{x} \tag{5.12}$$

Conversely, the primitive function of $1/x$ is $\ln x$.

5.4 Taylor Expansion

If $f(x)$ and all its derivatives are smooth functions of x, then we can write:

$$f(x+a) = f(x) + \left(\frac{\partial f}{\partial x}\right)_x a + \frac{1}{2!}\left(\frac{\partial^2 f}{\partial x^2}\right)_x a^2 + \cdots + \frac{1}{n!}\left(\frac{\partial^n f}{\partial x^n}\right)_x a^n + \cdots \tag{5.13}$$

The first two terms in the Taylor expansion are often used to approximate $f(x+a)$ if a is sufficiently small

$$f(x+a) \approx f(x) + \left(\frac{\partial f}{\partial x}\right)_x a$$

Specific examples are:

$$\begin{aligned}
\exp(x) &\approx 1 + x \\
\ln(1+x) &\approx x \\
\sqrt{1+x} &\approx 1 + \frac{1}{2}x \\
(1+x)^n &\approx 1 + nx \\
\sin(x) &\approx x
\end{aligned}$$

where, in all cases, it has been assumed that $|x| \ll 1$. For functions of more than one variable, this can be generalized to

$$f(x_1 + \Delta x_1, x_2 + \Delta x_2, \cdots, x_n + \Delta x_n) \approx f(x_1, x_2, \cdots, x_n) + \sum_{i=1}^{n}\left(\frac{\partial f}{\partial x_i}\right)\Delta x_i \tag{5.14}$$

5.5 Geometric Series

Consider the sum

$$S = \sum_{i=0}^{n} a x^i \tag{5.15}$$

Clearly,

$$xS = \sum_{i=0}^{n} a x^{i+1} = S - a + a x^{n+1} \tag{5.16}$$

Hence

$$S(1-x) = a(1-x^{n+1}) \tag{5.17}$$

or

$$S = \frac{a(1-x^{n+1})}{1-x} \tag{5.18}$$

If $|x| < 1$, we can take the limit $n \to \infty$

$$S_{n\to\infty} = \frac{a}{1-x} \tag{5.19}$$

so

$$\sum_{i=0}^{\infty} x^i = \frac{1}{1-x} \tag{5.20}$$

for $|x| < 1$. Differentiating both sides of Eq. 5.20 with respect to x and multiplying with x we get another useful expression

$$\sum_{i=0}^{\infty} i \times x^i = \frac{x}{(1-x)^2} \tag{5.21}$$

for $|x| < 1$.

5.6 Factorials and Permutations

The symbol $N!$ denotes the "factorial" of N. For positive, integer N, it is defined as

$$N! = N \times (N-1) \times (N-2) \times \cdots \times 2 \times 1 \tag{5.22}$$

In addition, $0! \equiv 1$. The number of permutations of a set of N labeled objects is equal to $N!$. This can be demonstrated by induction. The number of ways in which a single object can be ordered is clearly equal to 1, which is equal to 1!. Hence, the relation holds for $N = 1$. The next step is to show that if the relation holds for N objects, it also holds for $N+1$ objects. This is easily demonstrated as follows. Assuming that there are $N!$ permutations for N objects, then for every permutation there are $N+1$ positions in the sequence where we could insert object $N+1$. Hence the total number of permutations for $(N+1)$ objects is $(N+1) \times N! = (N+1)!$. This completes the proof.
Now consider the following question: we have N labeled objects and we wish to count the number of distinct ways that these objects can be divided into two sets, such that one set contains M elements and the other $N-M$ elements. For instance, 3 objects can be distributed in 3 ways over a subset of size one and a subset of size 2:

$$(1,2\,3), (2,3\,1)\ and\ (3,1\,2) \tag{5.23}$$

Note that we do not count different permutations within one subset as distinct. To compute this number in general, we consider all possible permutations of N objects. There are $N!$ such permutations. For every permutation, we attribute the first M elements to one set, and the remaining $N-M$ elements to the other. In this way, we get that the total number of permutations with M elements in one set and $N-M$ in the other is equal to $N!$. However, in this counting procedure, we have considered different permutations of the objects in either set as distinct. To get the total number of ways to distribute N objects over the two subsets, we should divide by the number of permutations in the set of M objects and in the set of $N-M$ objects. The result is that the number of ways to divide N objects over two subsets of size M and $N-M$ respectively, is given by the so-called binomial coefficient

$$\binom{N}{M} \equiv \frac{N!}{M!(N-M)!} \tag{5.24}$$

The binomial summation formula is

$$\sum_{M=0}^{N} \binom{N}{M} p^M q^{N-M} = (p+q)^N \tag{5.25}$$

The related expression

$$\sum_{M=0}^{N} M \binom{N}{M} p^M q^{N-M} = Np(p+q)^{N-1} \tag{5.26}$$

is obtained by differentiating both sides of Eq. 5.25 with respect to p and multiplying by p.

5.7 Binomial and Multinomial Distributions

As explained above, the number of ways to distribute N objects over two classes, in such a way that M objects end up in class I and $N-M$ objects in class II is given by

$$\frac{N!}{M!(N-M)!} \equiv \binom{N}{M} \tag{5.27}$$

For example: the number of ways to throw N coins, such that M are head and $N-M$ are tail, is $(N\ M)$. If we assume that the probability of head and tail are both equal to $1/2$, then the probability that I throw M heads and $N-M$ tails is

$$P(M,N-M)=\binom{N}{M}\left(\frac{1}{2}\right)^N \tag{5.28}$$

In the more general case that the probabilities for the two events are not equal - say the probability to throw head is p, then the probability to throw head M times and tail $N-M$ times is

$$P(M,N-M)=\binom{N}{M}p^M(1-p)^{N-M} \tag{5.29}$$

Of course, the sum of the probabilities of all different outcomes should add up to one

$$\sum_{M=0}^{N}\binom{N}{M}p^M(1-p)^{N-M}=(p+(1-p))^N=(1)^N=1 \tag{5.30}$$

To give a specific example, consider two containers, one with volume V_1 and the other with volume V_2. We assume that the probability that a molecule will be in volume 1 is equal to $V_1/(V_1+V_2)$. The probability to find a molecule in volume 2 is then $1-V_1/(V_1+V_2)=V_2/(V_1+V_2)$. The probability to find M molecules in V_1 and $N-M$ molecules in V_2 is then

$$P(M,N-M)=\binom{N}{M}\frac{V_1^M V_2^{N-M}}{(V_1+V_2)^N}. \tag{5.31}$$

The probability to find *all* molecules in volume 1 is

$$P(N,0)=\frac{V_1^N}{(V_1+V_2)^N} \tag{5.32}$$

In case we distribute N objects over a larger number of classes - say m - the number of realizations is given by

$$\frac{N!}{\prod_{i=1}^{m}M_i!} \tag{5.33}$$

where M_i is the number of objects in class i and

$$\sum_{i=1}^{m}M_i=N \tag{5.34}$$

5.8 Some Integrals

Certain integrals occur time and again in statistical mechanics. First of all, there are the integrals of the type:

$$\int_0^\infty dx\,x^n\exp(-ax) \tag{5.35}$$

All these integrals can be derived through integration by parts from the integral

$$\int_0^\infty dx\,\exp(-ax)=1/a \tag{5.36}$$

For instance

$$\int_0^\infty dx\, x\, \exp(-ax) = \Big[-\frac{x}{a}\exp(-ax)\Big]_0^\infty + \int_0^\infty dx\, \frac{\exp(-ax)}{a}$$
$$= \frac{1}{a^2} \tag{5.37}$$

The general result is

$$\int_0^\infty dx\, x^n\, \exp(-ax) = \frac{n!}{a^{n+1}} \tag{5.38}$$

This result can also be obtained by noting that

$$x^n\, \exp(-ax) = (-1)^n \left(\frac{\partial^n \exp(-ax)}{\partial a^n} \right) \tag{5.39}$$

and that therefore

$$\int_0^\infty dx\, x^n\, \exp(-ax) = (-1)^n \left(\frac{\partial^n (1/a)}{\partial a^n} \right) = \frac{n!}{a^{n+1}} \tag{5.40}$$

A second type of integral of particular importance is the Gaussian integral

$$I = \int_{-\infty}^\infty dx\, \exp(-cx^2) \tag{5.41}$$

A trick to compute this integral, is to consider its square

$$I^2 = \left(\int_{-\infty}^\infty dx\, \exp(-cx^2) \right)^2 = \int_{-\infty}^\infty dx\, \exp(-cx^2) \int_{-\infty}^\infty dy\, \exp(-cy^2) \tag{5.42}$$

We can write the latter product of integrals as

$$\int_{-\infty}^\infty dx\, \exp(-cx^2) \int_{-\infty}^\infty dy\, \exp(-cy^2) = \int_{-\infty}^\infty \int_{-\infty}^\infty dy\, dx\, \exp(-cx^2)\, \exp(-cy^2) \tag{5.43}$$

The latter integral is a two-dimensional integral. It can be simplified by using the polar coordinates r and ϕ, such that $x = r\cos\phi$ and $y = r\sin\phi$. Clearly, $x^2 + y^2 = r^2$. The integration range for ϕ is $\{0, 2\pi\}$ and r ranges from 0 to ∞. Finally, we replace the area element $dx\, dy$ by $r d\phi\, dr$. We can then write

$$\begin{aligned} I^2 &= \int_0^{2\pi} d\phi \int_0^\infty dr\, r\, \exp(-cr^2) \\ &= 2\pi \int_0^\infty \frac{1}{2} dr^2\, \exp(-cr^2) \\ &= \pi \int_0^\infty dr^2\, \exp(-cr^2) \\ &= \frac{\pi}{c} \end{aligned} \tag{5.44}$$

where, in the third line, we have used $dr^2 = 2r\, dr$. To arrive at the last equality, we used Eq. 5.36. Hence

$$\int_{-\infty}^\infty dx\, \exp(-cx^2) = \sqrt{\frac{\pi}{c}} \tag{5.45}$$

This means of course that

$$\int_0^\infty dx\, \exp(-cx^2) = \frac{1}{2}\sqrt{\frac{\pi}{c}} \tag{5.46}$$

Another useful expression is

$$\int_0^\infty dx\, x^{2n} \exp[-ax^2] = \frac{1 \times 3 \times 5 \times \cdots (2n-1)}{a^n 2^{n+1}} \sqrt{\frac{\pi}{a}} \tag{5.47}$$

5.9 STIRLING'S APPROXIMATION

In statistical thermodynamics the factor $N!$ often appears for very large values of N. Then one can consider N as a continuous variable and $N!$ as a continuous function of N that can be differentiated with respect to N. Stirling's approximation for $\ln N!$ is very often used. In its simplest form it is obtained from

$$\ln N! = \sum_{k=1}^{N} \ln k \approx \int_1^N dx \ln x = [x \ln x - x]_1^N = N \ln N - N + 1 \approx N \ln N - N \tag{5.48}$$

which is equivalent to

$$N! = \left(\frac{N}{e}\right)^N \tag{5.49}$$

Note that differentiation of Eq. 5.48 gives

$$\frac{d \ln N!}{dN} \approx \ln N = \ln N! - \ln(N-1)! \tag{5.50}$$

In some cases Eq. 5.48 is not accurate enough. From Eqs. 5.38 and 5.45 above, we can derive a better approximation for $N!$.

$$N! = \int_0^\infty dx\, x^N \exp(-x) = \int_0^\infty dx \exp(-x + N \ln x) \tag{5.51}$$

where we have used Eq. 5.38 with $a = 1$. The integrand is sharply peaked at $x = N$. The value of the exponent at $x = N$ is $-N + N \ln N$. The first derivative is zero (we are at a maximum). The second derivative is $-1/N$. Hence, we can approximate the integral by

$$\begin{aligned} N! &\approx \int_0^\infty dx \exp(-N + N \ln N - \frac{(x-N)^2}{2N}) \\ &= \int_{-N}^\infty du \exp(-N + N \ln N - \frac{u^2}{2N}) \end{aligned} \tag{5.52}$$

where we have defined $u \equiv x - N$. As the function is sharply peaked, we can replace the lower limit of the integration by $-\infty$. We then have

$$\begin{aligned} N! &\approx \exp(-N + N \ln N) \int_{-\infty}^\infty du \exp(-\frac{u^2}{2N}) \\ &= \exp(-N + N \ln N)\sqrt{2\pi N} \\ &= N^N \exp(-N)\sqrt{2\pi N} \end{aligned} \tag{5.53}$$

where we have used Eq. 5.45. This is Stirling's approximation for $N!$. In fact, Stirling's approximation is the first term of a series

$$N! = N^N \exp(-N)\sqrt{2\pi N}\left(1 + \frac{1}{12N} + \frac{1}{288N^2} - \frac{139}{51840N^3} + \cdots\right) \tag{5.54}$$

5.10 LAGRANGE MULTIPLIERS

Lagrange Multipliers can be used to find the minimum or maximum of a function $f(x_1, x_2, \cdots x_n)$ subject to the constraint $g(x_1, x_2, \cdots x_n) = 0$. Changes in f can be written as

$$df = \frac{\partial f}{\partial x_1} dx_1 + \frac{\partial f}{\partial x_2} dx_2 + \cdots + \frac{\partial f}{\partial x_n} dx_n \tag{5.55}$$

If all x_i would be independent, then all dx_i would be independent too and therefore this equation could be solved by setting each partial derivative

$$\frac{\partial f}{\partial x_i} \tag{5.56}$$

to zero. However, as $g(x_1, x_2, \cdots x_n)$ is kept constant, the x_i are no longer independent and the simple solution (all $\partial f/\partial x_i = 0$) is no longer valid. As $g(x_1, x_2, \cdots x_n)$ is kept constant, also

$$0 = dg = \frac{\partial g}{\partial x_1} dx_1 + \frac{\partial g}{\partial x_2} dx_2 + \cdots + \frac{\partial g}{\partial x_n} dx_n \tag{5.57}$$

Multiplying this equation by an unknown parameter λ and adding the two equations leads to

$$\left(\frac{\partial f}{\partial x_1} + \lambda \frac{\partial g}{\partial x_1}\right) dx_1 + \left(\frac{\partial f}{\partial x_2} + \lambda \frac{\partial g}{\partial x_2}\right) dx_2 + \cdots + \left(\frac{\partial f}{\partial x_n} + \lambda \frac{\partial g}{\partial x_n}\right) dx_n = 0 \tag{5.58}$$

The value of λ is chosen in such a way that

$$\frac{\partial f}{\partial x_n} + \lambda \frac{\partial g}{\partial x_n} = 0 \tag{5.59}$$

which means that

$$\left(\frac{\partial f}{\partial x_1} + \lambda \frac{\partial g}{\partial x_1}\right) dx_1 + \left(\frac{\partial f}{\partial x_2} + \lambda \frac{\partial g}{\partial x_2}\right) dx_2 + \cdots + \left(\frac{\partial f}{\partial x_{n-1}} + \lambda \frac{\partial g}{\partial x_{n-1}}\right) dx_{n-1} = 0 \tag{5.60}$$

Now the $n-1$ variables dx_i are independent, which implies that

$$\frac{\partial f}{\partial x_k} + \lambda \frac{\partial g}{\partial x_k} = 0 \tag{5.61}$$

for any $k = 1, 2, \cdots n$. The parameter λ is called the Lagrange multiplier. In practice one often first solves Eq. 5.61 first for all k, while treating λ as an unknown parameter, and then determines the value of λ such that the constraint $g(x_1, x_2, \cdots x_n) = 0$ holds for the solution that was found in that first step.

5.11 Dirac's delta function

Dirac's delta function $\delta(x)$ has the property

$$\int_{-\infty}^{\infty} dx f(x) \delta(x - a) = f(a) \tag{5.62}$$

and

$$\delta(x - a) = 0 \tag{5.63}$$

for $x \neq a$. The delta function of another function $g(x)$ is given by

$$\delta(g(x)) = \sum_i \frac{\delta(x - x_i)}{|g'(x_i)|} \tag{5.64}$$

in which the x_i are the solutions of $g(x_i) = 0$.

6 DEL

Let's invent a fake vector called $\vec{\nabla}$. The verbal name of ∇ is "del", standing, I suppose, for delta, although an honest delta is written as Δ. The components of $\vec{\nabla}$ are not numbers. They are derivative symbols:

$$\begin{aligned} \nabla_x &\equiv \frac{\partial}{\partial x} \\ \nabla_y &\equiv \frac{\partial}{\partial y} \\ \nabla_z &\equiv \frac{\partial}{\partial z} \end{aligned} \tag{6.1}$$

At first sight Equations 6.1 look like nonsense. The components of vectors are numbers, not derivative symbols. And anyway the derivative symbols don't make sense—derivatives of what? The point is that ∇ never stands alone. Just like the derivative symbol $\frac{d}{dx}$, it must act on something—it must have a function of some sort to differentiate. For example, ∇ can act on a scalar such as the temperature. The components of ∇T are

$$\begin{aligned} \nabla_x T &\equiv \frac{\partial T}{\partial x} \\ \nabla_y T &\equiv \frac{\partial T}{\partial y} \\ \nabla_z T &\equiv \frac{\partial T}{\partial z} \end{aligned} \tag{6.2}$$

and they indeed form the components of a genuine vector field—the gradient of the temperature. In a similar way, we can form the gradient of any scalar field.

Next, let's define the *divergence* of a vector field. The divergence is defined in analogy with the dot product of two vectors $\vec{V} \cdot \vec{A} = V_x A_x + V_y A_y + V_z A_z$, which, by the way, is a scalar. The divergence of a vector is also a scalar. Let the vector field be $\vec{A}(x)$. The divergence of $\vec{A}$ is the dot product of $\vec{\nabla}$ and $\vec{A}$—in other words, $\vec{\nabla} \cdot \vec{A}$. The meaning of this symbol is easy to guess by analogy with the usual dot product:

$$\vec{\nabla} \cdot \vec{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}.$$

7 PHASE SPACE FLUID

7.1 FLOW AND DIVERGENCE

Let's consider some simple examples of fluid flow in ordinary space. Forget about phase space for the moment, and just consider an ordinary fluid moving through regular three dimensional space labeled by axes x, y, z. The flow can be described by a *velocity field*. The velocity field $\vec{v}(x, y, z)$ is defined by going to each point of space and specifying the velocity vector at that point (see Figure 7.1).

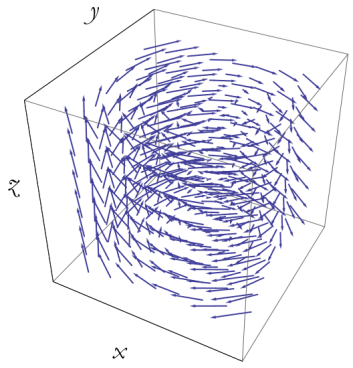

Figure 7.1: Velocity field.

Or we may describe the velocity field to be the components of the velocity: $v_x(x, y, z)$, $v_y(x, y, z)$, $v_z(x, y, z)$. The velocity at a point might also depend on time, but let's suppose that it doesn't. In that case the flow is called *stationary*.

Now let's suppose the fluid is incompressible. This means that a given amount of the fluid always occupies the same volume. It also means that the density of the fluid—the number of molecules per unit volume—is uniform and stays that way forever. By the way, the term incompressible also means indecompressible. In other words, the fluid cannot be stretched out, or decompressed. Consider a small cubic box defined by

$$x_0 < x < x_0 + dx$$
$$y_0 < y < y_0 + dy$$
$$z_0 < z < z_0 + dz.$$

Incompressibility implies that the number of fluid points in every such box is constant. It also means that the net flow of fluid into the box (per unit time) must be zero. (As many points flow in as flow out.) Consider the number of molecules per unit time coming into the box across the face $x = x_0$. It will be proportional to the flow velocity across that face, $v_x(x_0)$.

If v_x were the same at x_0 and at $x_0 + dx$, then the flow into the box at $x = x_0$ would be the same as the flow out of the box at $x = x_0 + dx$. However, if v_x varies across the box, then the two flows will not balance. Then the net flow into the box across the two faces will be proportional to

$$-\frac{\partial v_x}{\partial x} dx\, dy\, dz.$$

Exactly the same reasoning applies to the faces at y_0 and $y_0 + dy$, and also at z_0 and $z_0 + dz$. In fact, if you

add it all up, the net flow of molecules into the box (inflow minus outflow) is given by

$$-\left(\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+\frac{\partial v_z}{\partial z}\right)dx\,dy\,dz.$$

The combination of derivatives in the parentheses has a name: It is the *divergence* of the vector field $\vec{v}(t)$ and is denoted by

$$\nabla\cdot\vec{v}=\left(\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+\frac{\partial v_z}{\partial z}\right). \tag{7.1}$$

The divergence is aptly named; it represents a spreading out of the molecules, or an increase in the volume occupied by the molecules. If the fluid is incompressible, then the volume must not change, and this implies that the divergence must be zero.

One way to think about incompressibility is to imagine that each of the molecules, or points, of the fluid occupies a volume that cannot be compromised. They cannot be squeezed into a smaller volume, nor can they disappear or appear from nowhere. With a little bit of thought, you can see how similar incompressibility is to reversibility. In the examples that we examined in Lecture 1, the arrows also defined a kind of flow. And in a sense the flow was incompressible, at least if it was reversible. The obvious question that this raises is whether the flow through phase space is incompressible. The answer is yes, if the system satisfies Hamilton's equations. And the theorem that expresses the incompressibility is called Liouville's theorem.

8 THE VOLUME OF A HYPERSPHERE

In the following we derive the expression for the volume of a hypersphere of n dimensions. The volume is given formally by

$$V_n(R) = \int_{x_1^2+x_2^2+\cdots+x_n^2<R^2} dx_1\, dx_2 \cdots dx_n. \tag{8.1}$$

Because $V_n(R) \alpha R^n$ for $n = 2$ and 3, we expect that V_n is proportional to R^n. Hence, we write

$$V_n = C_n\, R^n, \tag{8.2}$$

where C_n is the unknown constant of proportionality which we wish to find. We rewrite the volume element $dV_n = dx_1\, dx_2 \cdots dx_n$ as

$$dV_n = dx_1\, dx_2 \cdots dx_n = S_n(R)\, dR = nC_n\, R^{n-1}\, dR, \tag{8.3}$$

where $S_n = nC_n\, R^{n-1}$ is the surface area of the hypersphere. For example, for $n = 3$ we have $dV_3 = 4\pi R^2 dR$ and $S_3 = 4\pi R^2$. To find C_n for general n, consider the identity

$$I_n = \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_n\, e^{-(x_1^2+\cdots+x_n^2)} = \left[\int_{-\infty}^{\infty} dx\, e^{-x^2}\right]^n = \pi^{n/2}. \tag{8.4}$$

The left-hand side of 8.4 can be written as

$$\begin{aligned} I_n &= \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_n e^{-(x_1^2+\cdots+x_n^2)} = \int_{-\infty}^{\infty} dR\, S_n(R)\, e^{-R^2} \\ &= nC_n \int_0^{\infty} dR\, R^{n-1}\, e^{-R^2}. \end{aligned} \tag{8.5}$$

We can relate the integral in 8.5 to the Gamma function $\Gamma(n)$ defined by the relation

$$\Gamma(n) = \int_0^{\infty} dx\, x^{x-1}\, e^{-x}. \tag{8.6}$$

The relation 8.6 holds for $n > -1$ and whether or not n is an integer. We make the change of variables $u = R^2$ so that

$$I_n = \frac{1}{2} nC_n \int_0^{\infty} du\, u^{n/2-1}\, e^{-u} = \frac{1}{2} nC_n\, \Gamma(n/2). \tag{8.7}$$

A comparison of 8.7 with 8.4 yields the desired relation

$$C_n = \frac{2\pi^{n/2}}{n\Gamma(\frac{n}{2})} = \frac{\pi^{n/2}}{(n/2)\Gamma(\frac{n}{2})} \tag{8.8}$$

It follows that

$$V_n(R) = \frac{2\pi^{n/2}}{n\Gamma(\frac{n}{2})} R^n. \tag{8.9}$$

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